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Our overall goal is to develop, implement and transfer accurate new numerical methods for solving the moving interface problems of solidification and crystal growth. We have several specific objectives: (1) Combine fast algorithms, level set techniques, adaptive refinement and data structures to develop and implement accurate, efficient and general new methods for moving sharp interfaces. (2) Develop a modular level set code for transfer to other researchers, labs and industry. (3) Combine spectral methods and stiff ODE solvers to produce fast spectrally-accurate solvers for phase field models of solidification and related problems. (4) Validate phase field models by numerical experiment and identify parameter choices appropriate to industrial settings.

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FINAL TECHNICAL REPORT

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Numerical Methods for Solidification Processes in Materials Science

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OBJECTIVES

Our overall goal is to develop, implement and transfer accurate new numerical methods for solving the moving interface problems of solidification and crystal growth. We have several specific objectives:

- Combine fast algorithms, level set techniques, adaptive refinement and data structures to develop and implement accurate, efficient and general new methods for moving sharp interfaces.
- Develop a modular level set code for transfer to other researchers, labs, and industry.
- Combine spectral methods and stiff ODE solvers to produce fast spectrally-accurate solvers for phase field models of solidification and related problems.
- Validate phase field models by numerical experiment and identify parameter choices appropriate to industrial settings.

STATUS OF EFFORT

We have attained our first and second objectives with the modular semi-Lagrangian methods for moving interfaces reported in Publications [P2–P5]. Our third objective was completed for the case of periodic boundary conditions in (Strain, 1995b), which is sufficient for basic validation and parameter identification. Further work on general boundary conditions and general domains is in progress. Additionally, we present efficient and accurate new vortex methods for convection in the melt in Publication [P1].

ACCOMPLISHMENTS AND NEW FINDINGS

We now summarize our progress in vortex methods and moving interfaces in more detail.

Vortex methods

We have studied vortex methods for incompressible 2D flows both as the simplest examples of level-set-based moving boundary techniques and as solvers for the convection in the melt around a growing crystal. Our most recent work on vortex methods is concisely surveyed in (Strain, 1996b).

- In 1992–4, we developed a new second-order accurate "triangulated" vortex method which solved the long-standing problem of long-time inaccuracy in traditional vortex methods (Russo and Strain, 1994).
- In 1994–5, we carried this line of research further. First, we developed an important tool for constructing quadrature formulas for singular integral operators in several dimensions (Strain, 1995a).

• Then in 1996, we produced new quadrature-based 2D vortex methods of arbitrary order with excellent long-time accuracy properties (Strain, 1996a).

• In 1996, we also developed new methods based on the smooth quadrature rules developed in (Strain, 1995a). Publication [P1] presents an accurate and efficient new approach to vortex methods for modeling incompressible inviscid fluid flow in two space dimensions.

Abstract

Since their introduction in the 1970's, vortex methods have been widely generalized and applied to compute many complex physical flows. They model such flows by moving discrete particles with a smoothed approximate fluid velocity. Thus their convergence analysis must balance smoothing errors against velocity approximation. Three long-standing theoretical problems have hampered the analysis of vortex methods:

- Long-time computations lose high-order accuracy via the Perlman effect: velocity approximation errors blow up when the flow map twists.
- Proofs of order-m convergence require $2m$ derivatives, much more than standard numerical methods.
- Parameter balances appropriate for convergence preclude efficient velocity evaluation by the fast multipole method.

Reformulation, quadrature and error analysis are used in this paper to solve these problems. The Perlman effect is eliminated by combining a free-Lagrangian formulation with fast adaptive quadrature rules. Thus long-time high-order accuracy is obtained by constructing a new set of particle weights at each step. A new error analysis of velocity approximation suggests a balance of parameters and choice of smoothing functions which requires only $m+1$ derivatives for essentially order-m convergence, halving the differentiability required of the flow. This balance can be combined with fast summation schemes to yield almost optimal efficiency. Numerical results verify the error analysis and exhibit excellent accuracy and efficiency, giving this approach—which generalizes widely—practical value as well as theoretical importance.

Summary

Vortex methods involve several components: velocity evaluation, vortex motion, diffusion, boundary conditions and regridding. In Publication [P1], we improve the speed, accuracy and robustness of the velocity evaluation. We eliminate the flow map, improve the quadrature used for the Biot-Savart law, and analyze the error in a nonstandard way, requiring less differentiability of the flow and obtaining efficient new parameter balances. We employ standard techniques for the vortex motion and consider inviscid free-space flow to eliminate diffusion and boundary conditions. Our approach combines naturally with regridding and fast summation methods.

First, we review Lagrangian vortex methods. These move the nodes of a fixed quadrature rule with the computed fluid velocity, preserving the weights of the rule by incompressibility. This procedure loses accuracy when the flow becomes disorganized, motivating many regridding techniques. Even before the flow becomes disorganized, however, obtaining high-order accuracy with a fixed quadrature rule requires smoothing of the singular Biot-Savart kernel. Smoothing gives high-order accuracy for short times but slows down fast velocity evaluation techniques and halves the order of accuracy relative to the differentiability of the flow. We review two free-Lagrangian vortex methods, the triangulated vortex method we developed in (Russo and Strain, 1994) and the quadrature-based method of (Strain, 1996a). Triangulated vortex methods are robust, practical and efficient but limited to second-order accuracy. Quadrature-based methods compute adaptive quadratures tailored to the Biot-Savart kernel at each time step, yielding long-time high-order accuracy at asymptotically optimal cost.

Publication [P1] develops a free-Lagrangian method which couples kernel smoothing with adaptive quadrature rules *not* tailored to the Biot-Savart kernel, producing long-time high-order accuracy. The asymptotic slowdown produced by kernel smoothing is almost eliminated by a careful choice of smoothing functions and parameters, based on a new error analysis of the velocity evaluation. This analysis requires about half as many derivatives of the solution as the standard approach.

The structure of our method is standard: At each time step, the smoothed velocity is evaluated once and the vortices are moved with an explicit multistep method. The velocity evaluation is nonstandard: First, a data structure groups the N vortices into cells convenient for integration. Then a global order-q quadrature rule is built. Finally, the fast multipole method is used with this rule to evaluate the smoothed velocity field.

The error is measured for standard test problems and our theoretical predictions are fully verified. Then more complex flows are computed.

Moving interfaces

Our work on moving interface problems in materials science combines fast PDE solvers such as boundary inte-

gral methods with fast geometric algorithms and level set techniques to build effective new numerical methods.

• In 1989, we developed a powerful implicit boundary integral method for computing periodic dendrite formation in a Stefan-type model of unstable solidification. We used a spectral discretization of a new arclength-preserving curve motion algorithm and an unconditionally-stable implicit time stepping scheme, solved by a modified Newton method. Our method was expensive but accurate and robust; higher-order accuracy was obtained by Richardson extrapolation. Numerical results agreed closely with linear stability theory and predicted correct tip-splitting phenomena in the nonlinear regime. The method and numerical results are presented in (Strain, 1989).

• In 1990, we developed fast algorithms for evaluating heat potentials (Greengard and Strain, 1990) which speeded up our boundary integral method (and many other calculations) by several orders of magnitude. This discovery led to the fast Gauss transform which has proven widely applicable (Greengard and Strain, 1991; Strain, 1991).

• In 1990–2, we developed a level set/boundary integral method for dendritic solidification (Sethian and Strain, 1992). This combined the boundary integral method of (Strain, 1989) with fast algorithms from (Greengard and Strain, 1990) and the level set method of (Osher and Sethian, 1988). The level set method handled topological changes effectively while fast boundary integral techniques ensured accuracy and efficiency in the velocity evaluation.

• In 1992–6, we developed efficient and accurate new vortex methods for modeling convection in the melt (Russo and Strain, 1994; Strain, 1996a), together with new error analyses [P1] and quadrature rules (Strain, 1995a) for general integral equations. Much of this work is summarized above and in (Strain, 1996b).

• Our major achievements in 1996–99 have been the development and implementation of highly effective new numerical methods for general moving interface problems. Abstracts of Publications [P2–P5], then an overview of these methods, follow.

Semi-Lagrangian methods for level set equations [P2]

A new numerical method for solving geometric moving interface problems is presented. The method combines a level set approach and a semi-Lagrangian time stepping scheme which is explicit yet unconditionally stable. The combination decouples each mesh point from the others and the time step from the CFL condition, permitting the construction of methods which are efficient, adaptive and modular.

Analysis of a linear one-dimensional model problem suggests a surprising convergence criterion which is supported by heuristic arguments and confirmed by an extensive collection of two-dimensional numerical results. The new method computes correct viscosity solutions to problems involving geometry, anisotropy, curvature and complex topological events.

Fast tree-based redistancing for level set computations [P3]

Level set methods for moving interface problems require efficient techniques for transforming an interface to a globally defined function whose zero set is the interface, such as the signed distance to the interface.

This paper presents an efficient algorithm for this "redistancing" problem. The algorithm uses trees and fast Delaunay triangulation to compute a global approximate signed distance function. An adaptive tree mesh is built to resolve the interface, and the vertex distances are evaluated exactly with an efficient search strategy, providing both continuous and discontinuous interpolants. Given a polygonal interface with N elements, the algorithm runs in $O(N \log N)$ space and time, and numerical results show it is highly efficient in practice.

Tree methods for moving interfaces [P4]

A fast adaptive numerical method for solving moving interface problems is presented. The method combines a level set approach with frequent redistancing and a semi-Lagrangian time stepping scheme which is explicit yet unconditionally stable. An adaptive tree mesh is used to concentrate computational effort on the interface, so the method moves an interface with N degrees of freedom in $O(N \log N)$ work per time step. Efficiency is increased by taking large time steps even for parabolic curvature flows. The method computes accurate viscosity solutions to a wide variety of difficult moving interface problems involving merging, anisotropy, faceting and curvature.

A fast modular semi-Lagrangian method for moving interfaces [P5]

A fast modular numerical method for solving general moving interface problems is presented. It simplifies code development by providing a black–box solver which moves a given interface one step with given normal velocity. The method combines an efficiently redistanced level set approach, a problem–independent velocity extension, and a second–order semi–Lagrangian time stepping scheme which reduces numerical error by exact evaluation of the signed distance function.

Adaptive quadtree meshes are used to concentrate computational effort on the interface, so the method moves an N–element interface in $O(N \log N)$ work per time step.

Efficiency is increased by taking large time steps even for parabolic curvature flows. Numerical results show that the method computes accurate viscosity solutions to a wide variety of difficult geometric moving interface problems involving merging, anisotropy, faceting, nonlocality and curvature.

Definitions and examples

A moving interface is a collection $\Gamma(t)$ of nonintersecting oriented closed curves (in the plane) or surfaces (in space). A sufficiently smooth moving interface has

- An outward unit normal vector $N(x,t)$,
- A signed curvature $C(x,t)$, and
- A normal velocity function $V(x,t)$.

A moving interface problem consists of a specification of $V(x,t)$ as a function of $\Gamma(t)$, its history and geometry, and any other fields or variables which may be present. For example, we may have passive transport

$$V(x,t) = N(x,t) \cdot F(x,t)$$

under a given velocity field F, or curvature- and angle-dependent normal velocity

$$V(x,t) = R + \epsilon \cos(k(\theta + \theta_0)) + \delta C$$

where $\cos\theta = N \cdot \hat{x}$, or we may have Stefan-type conditions such as

$$V(x,t) = \left[\frac{\partial u}{\partial N}\right]$$

where $u(x,t)$ solves the heat equation $u_t = \Delta u$ off $\Gamma(t)$ and $u = \epsilon C$ on $\Gamma(t)$, as in models for dendritic solidification of a pure material such as succinonitrile.

Level set equations

Any moving interface problem can be reformulated as a PDE for a function φ whose zero set is $\Gamma(t)$:

$$\Gamma(t) = \{x | \varphi(x,t) = 0\},$$

for example the signed distance function

$$\varphi(x,t) = \pm \min_{y \in \Gamma(t)} \|x - y\|$$

with the + sign chosen in the interior of $\Gamma(t)$. The normal, curvature and velocity are given by

$$N = \frac{\nabla \varphi}{\|\nabla \varphi\|},$$

$$C = -\nabla \cdot N,$$

$$V = \frac{\varphi_t}{\|\nabla \varphi\|}.$$

Level set methods

The level set method (Osher and Sethian, 1988) turns around the last formula for V and regards it as a PDE for φ:

$$\varphi_t - V\|\nabla \varphi\| = 0.$$

This requires us to extend V off $\Gamma(t)$ to a function defined everywhere. This "V extension" is one of the key ingredients of the level set technique. The V extension should be smooth and should agree with V on $\Gamma(t)$, but is otherwise arbitrary. The numerical properties of the method can be strongly affected by the choice of V extension.

The standard level set method involves four steps.

- Choose a V extension.
- Evaluate φ on a uniform mesh.
- Advance φ with a uniform mesh solver borrowed from hyperbolic conservation laws.
- Find $\Gamma(t)$ by contouring φ when desired.

A fifth step, redistancing, can be performed occasionally to enhance robustness:

- Replace φ by the signed distance to its zero set $\Gamma(t)$.

On a uniform mesh, redistancing can be extremely costly—as costly as the rest of the calculation put together.

Advantages and disadvantages

The main advantage of the level set method is *topological robustness*: merging and splitting pieces of interface is handled automatically by the level set equation. Potential disadvantages include the expense of going up a dimension, the grid-dependence of the solution, and the difficulty of finding a problem-dependent V extension. Since the method is explicit, tiny time steps are required for some problems. Stefan-type problems, for example, require the time step k to satisfy

$$k \leq O(h^3)$$

on a mesh of size h.

Our new method overcomes these disadvantages by combining the level set approach with an adaptive tree mesh for efficiency, a general problem-independent V extension, and an explicit unconditionally stable time stepping method.

Time stepping

Our time stepping method is based on the backward characteristic method of Courant, Isaacson and Rees (1952). The "CIR" method solves the hyperbolic equation

$$\varphi - F(x,t) \cdot \nabla\varphi = 0$$

by the following algorithm: At each x in the grid,

- Evaluate the velocity $F(x,t_n)$.
- Move x back with velocity $F(x,t_n)$ to $s = x+kF(x,t_n)$.
- Interpolate $\varphi(x,t_n)$ to the point s.
- Set $\varphi(x,t_{n+1})$ equal to the interpolated value.

The CIR method is first-order accurate and not in conservation form, but has the unusual property of being explicit yet unconditionally stable. It converges for model problems as long as

$$k \geq O(h), \quad .$$

an accuracy condition which is the reverse of the usual CFL stability condition.

We have developed a second-order "semi-Lagrangian" method which combines a CIR predictor

$$\tilde{\psi}(x) = \varphi(\tilde{x},t) = \varphi(x + kF(x,t),t) \qquad (1)$$

with a trapezoidal corrector

$$\psi(x) = \varphi(x + \frac{k}{2}F(\tilde{x},t) + \frac{k}{2}\tilde{F}(x,t+k),t). \qquad (2)$$

Here $\tilde{F}$ is built from the interfacial velocity $\tilde{V}$ of the zero set *Gamma* of the predicted solution $\tilde{\psi}$ at time $t+k$. This predictor–corrector pair is second-order accurate in time, explicit, and unconditionally stable; each time step requires two velocity evaluations. Since our advection velocity $F(x,t)$ extends the user-specified velocity functional V defined on the zero set $\Gamma(t)$ of $\varphi(x,t)$, each semi-Lagrangian time step requires several complex global operations. Starting with an interface $\Gamma(t)$, our method carries out the following steps to produce the new interface $\Gamma(t+k)$:

- Evaluate the signed distance φ from the interface $\Gamma(t)$.
- Evaluate the interfacial velocity V of $\Gamma(t)$ by a user-supplied module.
- Extend V to a global advection velocity F.
- Advance φ via F to the predicted CIR solution $\tilde{\psi}$ defined by Eq. (1).
- Contour $\tilde{\psi}$ to get the predicted interface $\tilde{\Gamma}$.
- Evaluate the predicted interfacial velocity $\tilde{V}$ of $\tilde{\Gamma}$.
- Extend $\tilde{V}$ to a global advection velocity $\tilde{F}$.
- Advance φ via F and $\tilde{F}$ to the corrected solution ψ defined by Eq. (2).
- Contour ψ to get $\Gamma(t+k)$.

Each of these steps can be efficiently implemented with an adaptive quadtree mesh.

Semi-Lagrangian methods for level set equations

We first tested the CIR scheme in Publication [P2] by solving level set equations with a fixed uniform mesh and ENO differencing, to obtain simplicity and high-order accuracy. We extended the velocity for passive transport and geometric moving interfaces by evaluating the natural formulas, with frequent redistancing, smoothing and truncation sufficient to satisfy the CFL condition even for parabolic problems like motion by curvature. A surprising result of this work is that the CFL condition can be satisfied by nonlocal velocity evaluation rather than restricting the time step. Numerical results verify the accuracy and stability of the method.

Fast tree-based redistancing for level set computations

As an intermediate step between the uniform mesh method and our ultimate goal, Publication [P3] develops an efficient new redistancing technique with the aid of a new data structure called the distance tree. This structure is a quadtree whose cells know their distance to $\Gamma(t)$ and nearby elements of $\Gamma(t)$, allowing for efficient approximate redistancing of φ. Figure 1 shows a pentagonal curve with the corresponding 6-level distance tree and signed distance function. The distance tree is built efficiently by a three-step recursive search procedure with guaranteed correctness. Delaunay triangulation is used to fix the sign of the signed distance function φ. The technique is asymptotically optimal, requiring only $(ON \log N)$ work to redistance an interface with N elements, and extremely fast in practice: computations of moderate complexity are speeded up 400 times, while redistancing the CIR calculation on a uniform mesh costs considerably less than moving φ one step.

Tree methods for moving interfaces

Our work with distance trees leads in to the adaptive tree-based level set method of Publication [P4]. Here we combine backward characteristics with an adaptive tree

mesh to build a method which is not only accurate and robust but also optimally efficient: An interface $\Gamma(t)$ with N degrees of freedom costs only $O(N \log N)$ to move one step. Efficiency is further enhanced by the semi-Lagrangian time stepping scheme: Large time steps can be taken even though the tree mesh contains tiny cells, because the backward characteristic method is unconditionally stable.

The tree mesh is refined with a new functional approach: Given a level set function $\varphi(x, t_n)$, we build a tree at time $t_{n+1} = t_n + k$ by recursive evaluation of $\varphi(x, t_{n+1}) = \varphi(s, t_n)$ at projected points $s = x + kF(x, t_n)$. The criterion for splitting a tree cell is simple: the values of $\varphi(x, t_{n+1})$ on the cell are smaller than the size of the cell. This contrasts favorably with standard mesh refinement algorithms, which tend to be based on error estimates for the computed solution.

In our numerical experiments, the velocity is evaluated either directly on the tree or by transferring φ to a uniform grid and employing the velocity evaluation technique of Publication [P2]. The sample calculations shown in Figure 2 clearly demonstrate the robustness of the tree method, even when computing complex merges between interfaces with corners. Grid effects, which often hamper level set methods, are clearly absent.

A fast modular semi-Lagrangian method for moving interfaces

A completely modular method for moving interfaces is developed and validated in Publication [P5]. It combines the ideas above with second-order semi-lagrangian time stepping, efficient exact quadtree-based redistancing, a modular problem-independent velocity extension, and exact φ interpolation in the semi-Lagrangian method. Our velocity extension technique evaluates the nearest-point extension on a distance tree, builds a continuous interpolant, and satisfies a maximum principle.

The modular method resolves and moves complex interfaces at optimal cost with time steps unconstrained by numerical stability. It is a "black-box" method for moving interfaces, which accepts the interface and its velocity at time t and returns the evolved interface one time step later. Such methods simplify moving interfaces, because the numerics are independent of the physical problem driving the interfacial motion.

Numerical results show that our method converges to correct viscosity solutions even for difficult moving interface problems involving merging, faceting, transport, nonlocality and anisotropic curvature-dependent geometry. Large time steps can be taken even for parabolic problems such as curvature flows. Selected computational results are shown in Figure 3.

PERSONNEL SUPPORTED

This grant has supported one faculty member (the PI) for the summer months of each academic year. The associated AASERT grant has supported one or more UC Berkeley graduate student per academic year: Ricardo Cortez (now an assistant professor at Tulane), Hans Johansen, Brandoch Calef and Paul Brown (now an assistant professor at the University of Illinois at Urbana-Champaign). The AASERT grant also funded a UC Berkeley undergraduate research project in wavelet analysis of PDEs, carried out by Jason Novotny (now in the graduate program at the Courant Institute).

PUBLICATIONS

Full texts of the following preprints are available at `http://www.math.berkeley.edu/~strain/`.

[P1] J. Strain. Fast adaptive 2D vortex methods. *J. Comput. Phys.*, 132: 108–122, 1997.

[P2] J. Strain. Semi-Lagrangian methods for level set equations. *J. Comput. Phys.*, 151:498–533, 1999.

[P3] J. Strain. Fast tree-based redistancing for level set computations. *J. Comput. Phys.*, 152:664–686, 1999.

[P4] J. Strain. Tree methods for moving interfaces. *J. Comput. Phys.*, 151:616–648, 1999.

[P5] J. Strain. A fast modular semi-Lagrangian method for moving interfaces. *J. Comput. Phys.*, submitted June 1999, revised January 2000.

INTERACTIONS AND TRANSITIONS

Conferences, meetings, seminars

Work supported by this grant was presented in the Computational Fluid Dynamics Workshop of the ASME Fluids Engineering Division Summer Meeting, San Diego, California, July 1996, and at seminars and colloquia at Argonne National Laboratory, Brown University, California Institute of Technology the University of Akron, the University of Chicago, the University of California at Berkeley, and Texas A&M University. The PI also gave a series of lectures in the Graduate Summer Course on Algebra, Algorithms and Approximation, at the Mathematical Sciences Research Institute, Berkeley, CA, July 1996.

Consultative and advisory functions

The PI served on the NSF/DARPA review panel for the Virtual Integrated Prototyping Initiative for Thin Films during September 1996, the first DARPA/NSF workshop

on Optimized Portable Application Libraries during June 1997, and the second DARPA/NSF workshop on Optimized Portable Application and Algorithm Libraries during December 1997. He also reviewed proposals for AFOSR and NSF, reviewed papers for Applied and Computational Harmonic Analysis, the Journal of Computational Physics, the Journal of Mathematical Analysis and Applications, the Monthly Weather Review, Proceedings of the Royal Society of London (Series A), and the SIAM Journal on Scientific Computing, and served as an Associate Editor of the SIAM Journal on Scientific Computing.

Transitions

The triangulated vortex method (Russo and Strain, 1994) developed under prior AFOSR support (Grant No. FDF-49620-93-1-0053) has been adopted by Dr. John Grant's group at the Naval Undersea Weapons Center, Newport, RI. They have applied the method to calculate moderate-Reynolds-number flows around various bodies of DoD interest and are currently extending the method to three-dimensional flows with boundaries.

The Ewald summation technique (Strain, 1992) developed under prior AFOSR support has been adopted by Dr. Raz Kupferman at Lawrence Berkeley National Laboratory as part of a new random vortex code he is developing.

NEW DISCOVERIES OR PATENTS

None.

HONORS AND AWARDS

The PI received a five-year NSF Young Investigator Award in September 1992.

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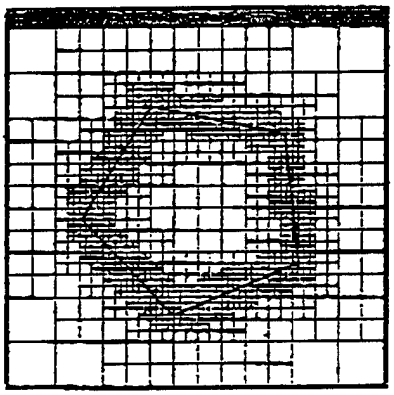

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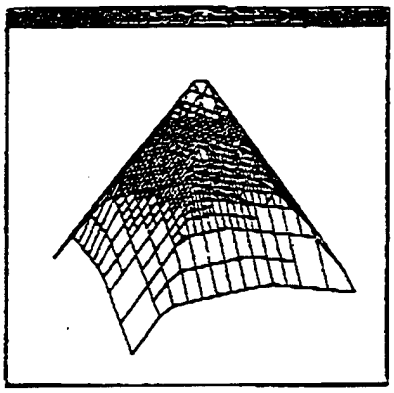
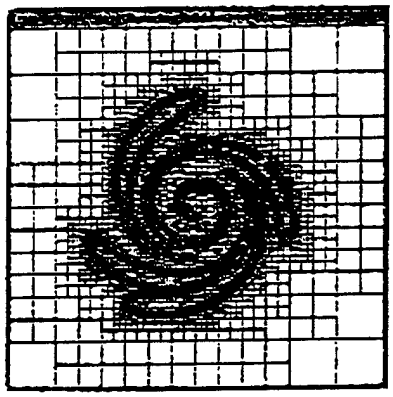


b

Figure 1: Six-level distance tree (a) and level set signed-distance function on tree (b).



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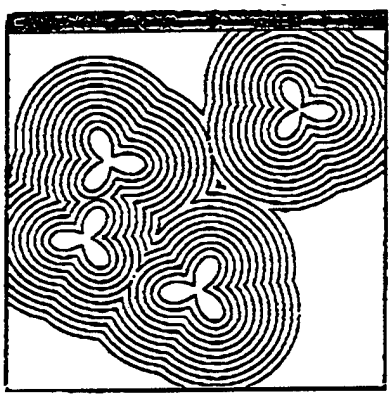

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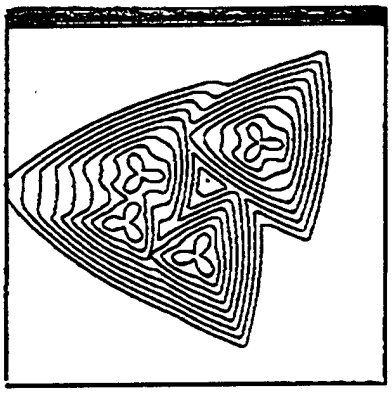

c

Figure 2: Sample solutions of moving interface problems: (a) initially circular bubbles after transport in a shearing flow, (b) merging of complex interfaces with unit normal velocity, and (c) crystalline facets developing under a threefold anisotropic curvature-dependent normal velocity.

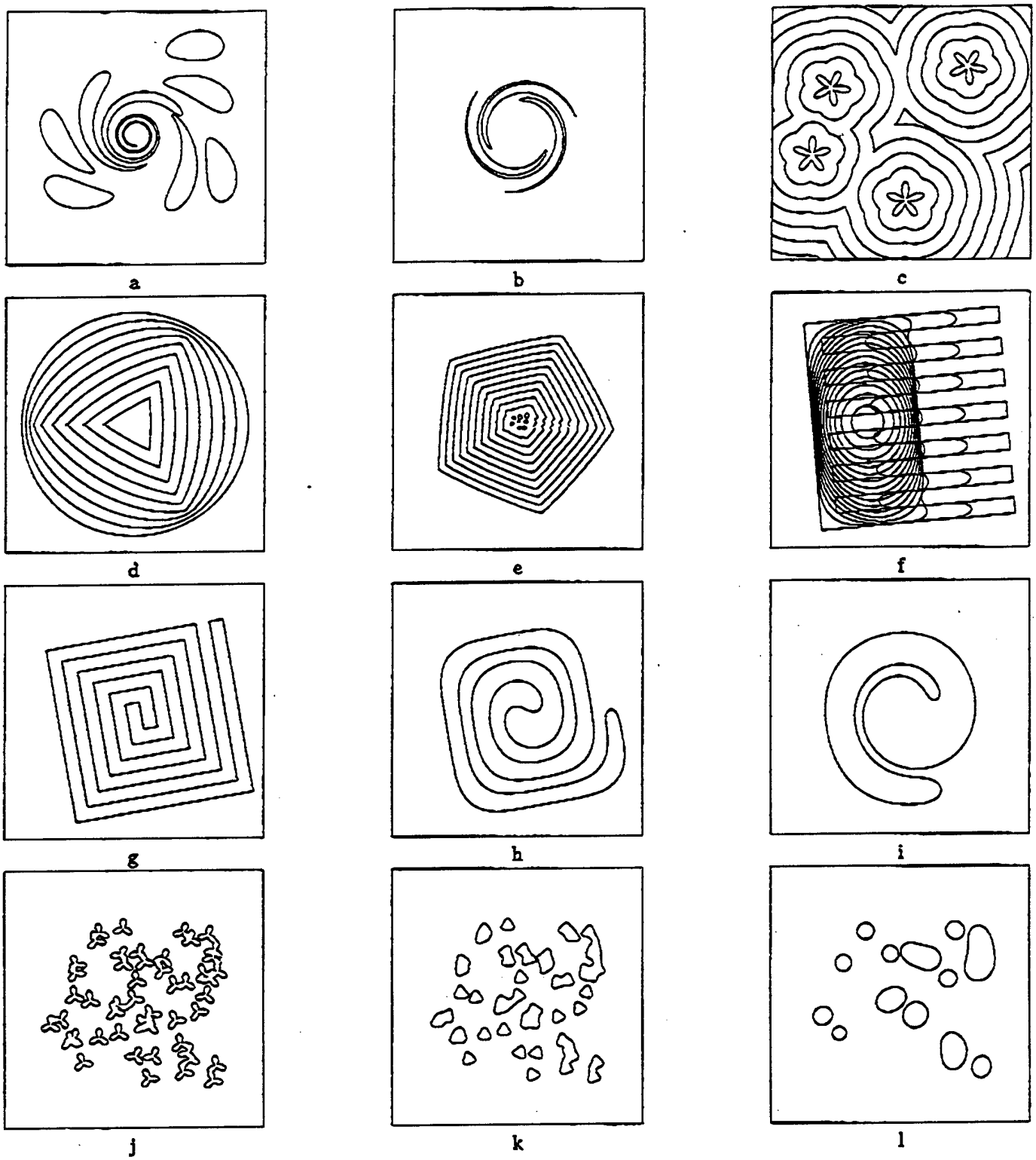

Figure 3: Selected computational results: (a-b) passive transport, (c) unit normal velocity, (d-e) shrinking and merging into Wulff shapes, (f) curvature flow, (g-i) spiral and (j-l) trefoils under volume-preserving curvature flow.